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Optimizing 3D Representations of Organic Processes.

James Hole
Fort Hays State University, jmhole@mail.fhsu.edu

Krisztina Bencze
Fort Hays State University, kzbencze@fhsu.edu

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James Hyun, James Hole, Dr. Krisztina Bencze, and Dr. Gordon Carlson
Fort Hays state University, Department of Chemistry, Department of Communication studies

Abstract

By minimizing the amount or processing that a computer must perform, the work and strain placed on that computer is greatly lessened. 3D representations of more complicated processes such as the visualization of the phospholipid bilayer described in “3D Modeling of Cellular Structures,” by Oo Hyung Jang, is an example of one of these 3D representations. The project created in the project is somewhat refined in this poster. This is accomplished by discarding unnecessary objects and pairings, extra faces, and extra codes. This will the lower the amount of objects that the computer will deal with, also lowering the total amount of work done by the computer.

Introduction

Utilizing newer technologies and software, representations of Chemical and Biological processes can be created in such as way that could not have been produced more than 15 years ago. In a previous poster, titled “3D Modeling of Cellular Structures,” made by Oo Hyung Jang, a process for creating a 3D representation of a cellular membrane is described. This process utilizes several different software and ends in a program called Unity which was originally created for video game design. The result of their research was an accurate representation of a biological process, but it had flaws. While a expensive, powerful computer, such as the ones housed in the Fort Hays State University New Media Lab, can run the program with little to no trouble, small and cheap computers cannot without ‘lagging,’ or having trouble processing the program causing the visual display to fall behind, create small gaps, or ‘lags’ in the middle of the display. The purpose of this poster is to explain what changes were made in order to make 3D representations, such as the one described in “3D Modeling of Cellular Structures,” more widely available.

Methodology

Overall, the method for this research will be the same as in “3D Modeling of Cellular Structures.” To start, using ChemSketch, a program created to help scholars create accurate representation of organic molecules more easily, the desired molecule is created and saved in the MDL format. Then, using a molecule converter extension in SketchUp, a 3D modeling program, the sketch of the molecule is converted into a malleable 3D object. This is where the methods begin to differ. Previously, the molecule was adjusted to the right scale and position, and then exported as a 3D object. Now, the molecule is scaled and adjusted, and then the Explode function is used until there is a single solid outline, upon which the Intersect Faces command would be used. The molecules would then be exported in the same manner as before. Once the molecules are objects inside of unity, the method differs once again. Originally, the molecules were assigned a script of code, which would instruct the molecules how to behave, where to move, etc. Then the molecules were saved as a “prefab,” which is a way of saving an object and its attachments, such as scripts, in a way that allows for multiple copies of that object to be accessed easily. There would then be a controller object that would a code create multiple molecules with attached scripts. After the code has started and the objects have been inserted in, the molecules would begin moving according to each individual code, creating the 3D representation of the process. The method used in this research is to first set the molecules as prefabs without having the code attached to each individual molecule. Then, a controller object would be created with two codes attached; one which would create all of the prefab molecules, and one which would control all of the movements of said molecules. See Figure 2 for pictures of this script. In the end, both methods create a working 3D representation of organic process.

Results

The previous method of creating the 3D representation had 3D objects, with multiple meshes, which determine the faces of the objects, as well as multiple objects within each object. Each individual component had its own object file as well as connection to other objects. The more recent method creates 3D objects with a single mesh and a single object per type of component as opposed to one object per individual component.

The previous method of coding started the same as the current method, with a controller object instantiating, or inserting, all the molecule in specified locations. Each instantiated object had scripts controlling that specific molecules movement which would operate independent of the other molecules. The current method has the controller object determine how the molecules will move with a single script instead of multiple.

Discussion

Using the current method should provide a noticeable increase in computer efficiency as well as decrease in lag, assuming that the computer being run is not a high-performance computer. This is due to the current process lowering the amount of work that the computer is needing to perform by a fairly substantial margin. The main part of this is in the SketchUp portion of the research. Before the Explode and Intersect faces are used, there are tens of thousands of faces, or small geometric shapes, that make up the object as well as all of the individual components. By exploding and intersecting the faces of the object, the molecules becomes one singular object instead of a parent object with multiple children objects and has only a few thousand faces to deal with. By making the molecule one single object, the computer will only see the individual molecule, rather than the entire molecules with all of the atoms and bonds included. When the scripts inside of Unity are applied to an object that hasn’t been exploded and intersected, the script will apply to the whole of the object, then all of the individual components and faces. By taking away the components and a significant portion of the faces, the amount of processing that the computer has to do goes down significantly. This is continued when the scripts are changed inside of Unity.

By using a single controller to move all of the molecules as opposed to a script for each individual molecule, the amount of processing needed to be done by the computer lessens. This is due to how the computer would interact will each object and their scripts. Originally, the computer, while running the scripts, would have to go to each object, read the code, and then move the molecule. The computer would have to take the time and processing power to read each individual code and then decide what to do with each object, despite the fact that they are all similar or even the same. By having one single code that controls each molecule, the amount of processing time goes down significantly because the process for the computer would be read the code, move the object, move the next object, etc. This would not only require the computer to only read one single, albeit slightly longer, script, but it also wouldn’t have to process what to do with each object as it would know do to the universally applied script that all of the molecules would be moved the exact same way. Overall, the amount of processing and time needed by the computer should be lowered enough that more standard or low performance computers should be able to run this 3D representation, allowing a greater number of people to access visual models of organic processing.

However, due to poor circumstances, including ill-matching schedules and the closing of Fort Hays State University due to COVID-19, not all of the projects described in “3D Modeling of Cellular Structures” was able to be optimized for low-performance usage. As such, the discussions, results, and methods of this poster only apply to a limited portion of the former research.

Figure 2

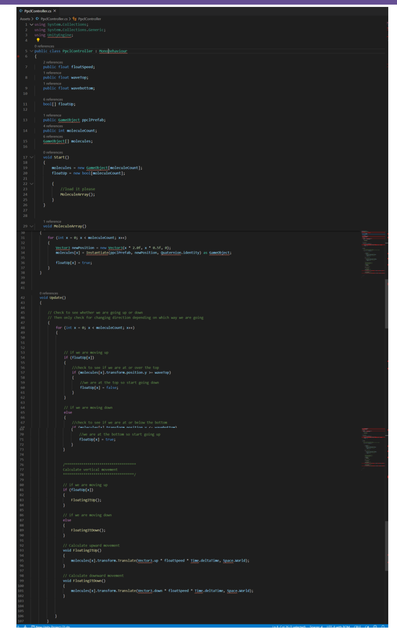

Figure 1: A series of three screenshots of the script written for the current form of the wave motion.

Conclusions

The methods described in this poster has decreased the amount of work needed to be done by a computer in order to successfully run our program, which should allow a larger variety of people to have access to this representation, as they would be less limited by their technology.

By utilizing the current methods, more 3D representations could be changed so that scholars with less access to high-performance technology could have access to visuals for occurrences not necessarily connected to organic processes.

Acknowledgements

Jang, Oo Hyang, (2018). 3D Modeling of Cellular Structures.
FHSU Institute for New Media Studies,
FHSU Department of Chemistry,
FHSU Department of Communications.